Modelling nanoparticle transport in porous media across the scales: from pore network models to simulation of filed injection

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Abstract (maximum: 4000 characters)

Transport and deposition of colloidal particles in saturated porous media are of great importance in many fields of science and engineering. A thorough understanding of particle filtration processes is essential for predicting the transport and fate of colloidal particles in the subsurface environment. Particles migrating through a porous medium can remain in suspension and be transported due to advection and dispersion phenomena, or be retained due to filtration and deposition onto the porous matrix. In particular, in the framework of the FP7 project Nanorem (G.A. Nr. 309517), the application of nanoparticles for groundwater remediation is the key research question. Colloid transport is a peculiar multi-scale problem, and pore-scale processes have an important impact on the transport at the larger scale. In this study, colloid transport modelling was carried out at different scales, from the pore scale (applying pore-network models) up to the full field scale. Assessing the mechanisms that control the mobility of reactive nanoparticles is of pivotal importance in the design, implementation, and performance evaluation of field applications. While numerical models for the simulation of dissolved contaminants transport are widely available, field scale models of nanoparticles with proven predictive ability are yet to be developed. This is mainly because the fundamental controlling mechanisms for the transport of nanoparticles in the subsurface at the field scale are not well understood.

Using pore network modelling we simulate fluid flow and transport of colloids within a network of interconnected pores (Raoof et al., 2013). Colloidal processes such as deposition and aggregation are implemented at the scale of individual pores. Averaging over the network domain composed of several pores, we derive macro-scale parameters to be used within field scale models (Raoof et al., 2010).

Transport of concentrated nanoparticle suspensions in porous media is affected by the rheological properties of the dispersing fluid (shear thinning) and by particle deposition and filtration in the porous matrix, which result in porous medium clogging (i.e. reduction of porosity and permeability). Moreover, the kinetics of particle retention is strongly influenced by the ionic strength of the pore water. Up to date, modelling of colloid transport in the presence of such complex interaction phenomena has been mainly faced in one-dimensional Cartesian coordinates for the simulation of laboratory column tests (Tosco et al., 2009; Tosco and Sethi, 2010), or at larger scales in simplified radial domains (Tosco et al., 2014), as implemented in MNMs (www.polito.it/groundwater/software/MNMs.php). In this work, a modelling tool for the

simulation of colloid injection and transport under transients in ionic strength in more complex scenarios is developed and validated. To this aim colloid transport equations were implemented in the well-known transport model RT3D (Clement et al., 1998). The tool can be used for multi-dimensional simulations, and the approach is validated through comparison of results from MNMs and RT3D for a one-dimensional domain.

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